Electrostatics / Poisson equation

\[ V = 0 \quad \text{V} \quad \text{V} = \alpha \]

\[ N_0 \]

\[ 0 \quad L \]

\[ N_0 \text{ doping profile of semiconductor (N-type)} \]

Find electrostatic potential \( V(x) \) solution of 1D Poisson equation

\[
- \frac{d^2 V(x)}{dx^2} = \frac{P(x)}{\varepsilon_S} \quad \text{charge density}
\]

\[
\text{Assumption} \quad P(x) = q N_0(x) \quad q = \text{electrical charge}
\]

\[
\forall x \in [0, L] \quad P(x) = q N_0 \quad \text{No uniform and known}
\]
\[ -\frac{d^2 V(x)}{dx^2} = \frac{qN_0}{\varepsilon_0} \quad x \in [0, L] \]

**Dirichlet boundary condition**

\[ V(0) = 0, \quad V(L) = L \]

One can show that this problem is well-posed

\[ \Rightarrow \text{existence/ uniqueness of solution} \]

\[ [\text{Lax - Milgram theorem}] \]

**Analytical treatment**

\[ -\frac{d^2 V(x)}{dx^2} = \frac{qN_0}{\varepsilon_0} \]

\[ \int_{0}^{L} V(x) \, dx = \frac{qN_0}{2\varepsilon_0} x + \frac{c_1}{2} \]

\[ V(0) = 0 \Rightarrow c_2 = 0 \]

\[ V(L) = L \Rightarrow c_1 = \left( \frac{qN_0 L^2 + \frac{\varepsilon_0}{2}}{2\varepsilon_0} \right) \]

\[ \Rightarrow V(x) = -\frac{qN_0}{2\varepsilon_0} \left[ x^2 - \frac{Lx}{2} \right] + \frac{Lx}{2} \quad x \in [0, L] \]
The price to pay for an analytical treatment is an over-simplification of the physical assumptions. Here, we assumed a simple uniform doping profile.

To go beyond the notion of "toy model" and toward "realistic" modeling, we need to resort to numerical modeling.
we propose to make use of the finite difference method (FDM) to discretize the equations ⇒ "numerical discretization"

Continuum space ⇒ Discretized space

\[ V(x) \times \in [0, L] \Rightarrow \{ V_i \} \quad i = 1, 2, \ldots, N \]

⇒ \( V(x) \) will only be computed at \( x = x_1, \ldots, x_n \)

\[ V(x_i) = V_i \quad \text{also} \quad p(x_i) = P_i \quad \text{(known)} \]

⇒ Problem equation at \( x = x_i \) (given position)

\[
-\frac{d^2 V(x)}{dx^2} = \frac{P_i}{\varepsilon s} \quad \forall i \in [1, \ldots, N]
\]

⇒ \( N \) equations
FDH approximation consists of replacing the operator of derivation by a discrete one.

\[ \text{discretization of the operator on a grid} \]

We also suppose an uniform grid, with the step \( a = \frac{|x_{i+1} - x_i|}{h} \).

With \( a \) small enough, one can use a Taylor development at \( x = x_i \):

\[
\begin{align*}
V_{i+1} &= V_i + \frac{a}{h} V'_i + \frac{a^2}{2} V''_i + O(a^3) \\
V_{i-1} &= V_i - \frac{a}{h} V'_i + \frac{a^2}{2} V''_i + O(a^3)
\end{align*}
\]

Using both equations (subtract them), one gets the central difference approximation:

\[
V'_i = \frac{V_{i+1} - V_{i-1}}{2a}
\]
By adding both equations, we get the equation

\[ V_i'' = \frac{1}{a^2} [V_{i+1} + V_{i-1} - 2V_i] \]

The new discretized Poisson equation looks like

\[ -\frac{1}{a^2} [V_{i+1} + V_{i-1} - 2V_i] = \frac{e_i}{\varepsilon_0} \quad \forall i \in \{1, N\} \]

we note that \( \int V_i = 0 \) from DBC

\( V_N = 0 \)

So we get \( N-2 \) equations, \( N-2 \) unknowns

System of equations

\[ \begin{align*}
-V_3 + 2V_2 &= \frac{a^2 \rho_2}{\varepsilon_0} \\
-V_4 - V_2 + 2V_3 &= \frac{a^2 \rho_3}{\varepsilon_0} \\
&\vdots \\
-V_2 + 2V_1 &= \frac{a^2 \rho_{N-1}}{\varepsilon_0} + x
\end{align*} \]
Linear system in matrix form

\[
\begin{bmatrix}
2 & -1 \\
-1 & 2 & -1 \\
-1 & 2 & -1 \\
\end{bmatrix}
\begin{bmatrix}
V_2 \\
V_3 \\
V_{n-1}
\end{bmatrix}
= 
\begin{bmatrix}
p_2 a^{2/5} \\
p_3 a^{2/5} \\
\text{etc.} + 2
\end{bmatrix}
\]

\[
\mathbf{A} \cdot \mathbf{X} = \mathbf{B}
\]

Remark: We have transformed a 1D problem along \( x \) into a \((N-2)\) dimensional problem!
But it can now be solved numerically.

Numerical approximation depends on the step \( a \).
\[
\lim_{a \to 0} \left( \text{True Solution} - \text{Numerical Solution} \right) = 0
\]
Replace all matrix-vector elements by their numerical values. We are using a numerical algorithm for solving

\[ A \mathbf{x} = \mathbf{b} \quad \Rightarrow \quad \text{Linear System} \]

Matrix \quad \text{solution} \quad \text{Right-hand-side (RHS)}

Remarks:

- \( A \) is positive definite (explain later in class)
  
  So "invertible", well-conditioned matrix.

- Direct inversion of \( A \) \[ \text{computing explicitly } A^{-1} \]
  is always too expensive numerically.

- Direct methods use "Gaussian elimination" and other "LU" decomposition technique.

Most numerical libraries offer such routines.

Example: MATLAB \( A \backslash \mathbf{b} \)
However, $A \backslash B$ is "hiding" the computing kernel.

The kernel of linear algebra routines is

\[ \text{LAPACK} \Rightarrow \text{a suite of highly optimized linear algebra routines} \]

linear Algebra package [that can be called from C or Fortran (in particular)]

Let us now consider a dense storage for $A$ and $B$ where all zeros are stored.

[Note: $A$ is tridiagonal, we could save memory by not storing all elements.]

One routine to be called (for example)

\[ \text{GESV} \begin{bmatrix} N, NRHS, A, DA, IPIV, B, LDB, INFO \end{bmatrix} \]

solution

\[ X = SD \Rightarrow \text{single/double real} \]
\[ = C, Z \Rightarrow \text{single/double complex} \]
In our example one could use DGESV

\[ N \leq N-2 \quad \text{"size"} \]

\[ NRHS \leq 1 \quad \text{"1 RHS"} \]

\[ LDA \leq N-2 \quad \text{"physical size" suffix leading dimension} \]

\[ LDB \leq N-2 \quad \text{"physical size" suffix} \]

\[ A \text{ is a N-2 x N-2 array (double real)} \]

\[ B \text{ is a N-2 vector (double real)} \]

\[ \text{IN1N is a "work array", integer array size N-2} \]

\[ \text{INFO is an integer} \]

\[ \text{INFO return } 0 \text{ is everything is fine} \]

\[ B \text{ contains the solution vector X on exit}. \]

Remark: The accuracy of the solution depends also on the computing arithmetic precision (floating point arithmetic).

Example: [double precision \( \approx 16 \) digits accuracy \((10^{-16})\)]

[Single precision \( \approx 7 \) digits \((10^{-7})\)]
memory requirements

Real  single  4 byte,
Integer  2 byte,
Double  8 byte.

Complex = 2 x Real

Simulation of solution vector

\[ X = \begin{bmatrix} V_2 \\ V_3 \\ \vdots \\ V_n \end{bmatrix} \] can be plotted

It becomes easy to modify values of f(x) \([\text{RHS} B]\) and solve again the linear system.